Published in final edited form as:

J Biomech Eng. 2010 October ; 132(10): 101001. doi:10.1115/1.4002371.

RADIAL TRANSPORT ALONG THE HUMAN ACINAR TREE

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Abstract

A numerical model of an expanding asymmetric alveolated duct was developed and used to investigate lateral transport between the central acinar channel and the surrounding alveoli along the acinar tree. Our results indicate that some degree of recirculation occurs in all but the terminal generations. We found that the rate of diffusional transport of axial momentum, from the duct to the alveolus, was by far the largest contributor to the resulting momentum in the alveolar flow but that the magnitude of the axial momentum is critical in determining the nature of the flow in the alveolus. Further, we found that alveolar flow rotation, and by implication chaotic mixing, are strongest in the entrance generations. We also found that the expanding alveolus provides a pathway by which particles with little intrinsic motion can enter the alveoli. Thus, our results offer a possible explanation for why submicron particles deposit preferentially in acinar entrance region.

INTRODUCTION

The human lung contains several hundred million small gas exchange units – called alveoli. Respiratory gases, such as O₂ or CO₂, are transported from the alveolar opening to the gas-exchange surface predominantly by molecular diffusion. In contrast, those aerosol particles that reach the gas exchange region of the lung have little intrinsic motion (i.e., motion due to inertia, gravitational sedimentation, or diffusion) and are entrained, or convected, by the airflow patterns that exist inside the alveoli.

More than a decade ago, we set out to investigate airflow patterns in model alveoli in order to understand better alveolar particle transport. The flow in alveoli is driven by the motion of the expanding and contracting alveolar septal walls. We found that alveolar flow can rotate and be highly complex despite the fact that it is typically a slow viscous flow of low Reynolds number (Tsuda et al., [1]). The most surprising and intriguing implication of this finding is that alveolar flow can cause flow-induced, chaotic, mixing inside the alveoli and the alveolar ducts (Tsuda et al., [1, 2, 3]; Henry et al., [4, 5]; Haber et al., [6]). This discovery was fundamental for the following reasons: 1) it explained theoretically how inhaled aerosol particles can mix with residual alveolar air convectively rather than by any means attributable to the particles' intrinsic motion; 2) it implies that any alveolus within which the flow rotates can generate chaotic convective mixing. Thus, each alveolus with rotational flow has the potential to be an effective flow mixer.

The above result assumes that particles have easy access to the rotational flow in the alveoli. That is, for particles to be affected by this mixing mechanism they need first to enter the alveoli from the acinar central airways. Inhaled aerosol particles are transported axially from the environment to deep into the alveolar region of the lung via the respiratory tract. For those particles to enter the alveoli, which are dead-end side pockets, they need to be

transported across the main flow direction and through the alveolar opening. However, this lateral motion –a communication between the alveolar ducts and alveoli– is not well understood.

In the past, models of acinar flow considered the alveolar walls to be rigid but such models have a streamline separating the duct flow from that in the alveolus; this prevents any convective communication between these two regions. Consequently, rigid-walled models of alveolar particle transport cannot be considered physiologically realistic because the intrinsic motion of aerosol particles is too small to account for any appreciable rate of particles entering the alveoli. To overcome this limitation, we proposed the use of rhythmically expanding alveolar models (Tsuda et al., [1]; Haber et al., [6]; Henry et al., [4]) which were later adopted and studied by others (e.g., Lee & Lee [7]; Snitzman et al., [8]; Kumar et al., [9]; Darquenne et al., [10]). Such models allow radial convective communication, indicating that this type of model is more realistic and physiological.

The objective of this study is to investigate lateral transport between the central acinar channel and the surrounding alveoli along the acinar tree. We use our current moving-wall model, which is simple but complex enough to encapsulate the essence of this basic structure of the acinar airways. We concentrate on the fluid mechanics underlying the basic process because inhaled particles of interest enter the alveolus mostly by convection (i.e., they are carried in with the fluid which is drawn into the alveolus by its expansion), rather than by their own intrinsic motion (e.g., inertia, gravitational sedimentation, or diffusion).

THEORETICAL CONSIDERATIONS

The acinar, or respiratory, region of the lung is defined as starting at the transitional bronchioles; i.e., in the airways in which alveoli first appear. Transitional bronchioles are approximately 0.5 mm in diameter (d) and typically occur in generation 15 of the dichotomously bifurcating airway tree [11]. The acinus is generally agreed to have, on average, eight generations below the entrance generation; that is, the terminal alveolar sacs are located at generation 23 (Fig 1).

In normal breathing, we inhale approximately 500 ml of air over a period of two seconds [12]. At each bifurcation, the airflow rate is roughly divided by half and hence the average velocity of the air in an airway, U , quickly reduces and is less than 40 mm/s in the transitional bronchioles. Hence, the Reynolds number ($Re = Ud/\nu$, where ν is the kinematic viscosity) of the flow in the acinar-entrance airways is of order one and thus inertial effects are relatively unimportant. As the airways in the acinus also follow a bifurcating pattern, the Reynolds number further reduces by half in each subsequent acinar generation. The flow of air travels along the same pathways in inhalation and exhalation and hence the flow direction reverses completely over the breathing cycle. Nonetheless, the change in the flow over the breathing period is slow relative to the cross-stream viscous diffusional time ($d^2/\nu \approx 0.015$ s), and hence acinar flow is quasi steady. This is confirmed by the Womersley number ($\alpha = d\sqrt{2\pi f/\nu}$, where f is the frequency in hertz) being approximately 0.15. While lung flow is quasi steady, it is produced by the expansion and contraction of the lung volume, and thus the motion of the septal walls is a defining feature of acinar flow.

Fluid flow, in general, is governed by two conservation laws (assuming constant properties): the conservation of mass and the conservation of momentum. In this paper, we are principally interested in the communication between the flow in the central acinar airways and that in the alveoli. Thus, we are primarily concerned with the radial transport of mass and momentum. There are four components to the radial transport of momentum: (i)

convection of axial momentum; (ii) diffusion of axial momentum; (iii) convection of radial momentum; (iv) diffusion of radial momentum.

In the following, we perform an order-of-magnitude analysis of the relative importance of each of the four components of radial transport for each generation along the acinar tree over inspiration.

Radial diffusion of axial momentum

In the rigid case, diffusion is the only mechanism by which the axial momentum can enter the alveolus. However, regardless of whether or not the alveolus is expanding, the diffusional flux of axial momentum (per unit volume) in the radial direction, $-\nu (\rho u_z)/r$, scales as $\mu U/d$, where $U = 4Q_D/\pi d^2$ is the mean velocity in the duct, Q_D is the volume flow rate in the duct, and d is the duct diameter. Hence, integrating over the alveolar width, w , the rate at which axial momentum (per unit volume) diffuses radially into the alveolus is, approximately,

$$-\pi d \int_0^w [\nu \partial(\rho u_z)/\partial r] dz \approx \pi \int_0^w (\mu U) dz = \pi \mu U w = 4 \frac{\mu w}{d^2} Q_D \quad (1)$$

Radial convection of axial momentum

In the actual case, the alveoli expand and draw in both mass and momentum. We assume that the convective flux of axial momentum (per unit volume) in the radial direction, $\rho u_r u_z$, scales as $\rho V U$, where $V = Q_A/\pi d w$ and Q_A is the volume flow into the alveolus due to its expanding volume. Hence, the rate at which axial momentum (per unit volume) convects radially into the alveolus, over inspiration, can be approximated as

$$\pi d \rho \int_0^w (u_r u_z) dz \approx \rho \pi d \int_0^w U V dz = \rho \pi d U V w = \frac{4\rho}{\pi d^2} Q_A Q_D \quad (2)$$

The ratio of convection to diffusion of axial momentum, R_1 , is then

$$R_1 = \frac{1}{\pi \nu w} \frac{Q_A}{Q_D}$$

$$\text{or, as } \frac{1}{\nu} = \frac{\pi d \text{Re}}{4 Q_D}$$

$$R_1 = \frac{1}{4} \frac{d}{w} \frac{Q_A}{Q_D^2} \text{Re}$$

Radial diffusion of radial momentum

The diffusional flux of radial momentum (per unit volume) in the radial direction, $-\nu (\rho u_r)/r$, is assumed to scale as $\mu V/h$. Also, as $h = w$, we can write $-\nu (\rho u_r)/r \sim \mu V/w$. Hence, the rate at which radial momentum (per unit volume) diffuses radially into the alveolus can be approximated as

$$-\pi d \int_0^w (v \partial(\rho u_r)/\partial r) dz \approx \pi d \int_0^w (\mu V/w) dz = \pi d (\mu V/w) w = \mu \frac{Q_A}{w} \quad (3)$$

The ratio of diffusion of radial momentum to diffusion of axial momentum, R_2 , is then

$$R_2 = \frac{\mu \frac{Q_A}{w}}{4 \frac{\mu w}{d^2} Q_D} = \frac{1}{4} \left(\frac{d}{w} \right)^2 \frac{Q_A}{Q_D}$$

Radial convection of radial momentum

We assume that the convective flux of radial momentum (per unit volume) in the radial direction, $\rho u_r u_r$, scales as ρVV . Hence, the rate at which radial momentum (per unit volume)) convects radially into the alveolus, over inspiration, can be approximated as

$$\pi d \rho \int_0^w (u_r u_r) dz \approx \pi d \rho \int_0^w (VV) dz = \pi d \rho V^2 w = \frac{\rho}{\pi d w} (Q_A)^2 \quad (4)$$

The ratio of convection of radial momentum to diffusion of axial momentum, R_3 , is then

$$R_3 = \frac{\frac{\rho}{\pi d w}}{4 \frac{\mu w}{d^2} Q_D} = \frac{d}{4 \pi \nu w^2} \frac{(Q_A)^2}{Q_D}$$

or, substituting for viscosity,

$$R_3 = \frac{1}{16} \left(\frac{d}{w} \right)^2 \left(\frac{Q_A}{Q_D} \right)^2 \text{Re}$$

The curves of R_1 , R_2 , and R_3 (Fig. 2) show that diffusion of axial momentum dominates the radial transport process for all but the most distal of generations. At the terminal generation, the rates of diffusion of axial and radial momentum are of equal magnitude. Conversely, throughout the acinus, radial convection of momentum from the duct to the alveolus is always negligible. It should be emphasize that while radial convection of momentum appears to be negligible, the air that enters the expanding alveolus, due to the requirement of conservation of mass, is the only pathway for particle-laden tidal air to enter the alveolus.

NUMERICAL METHODS

Model geometry

The model comprises three identical annular alveoli in axial alignment (Fig. 3a). Each alveolus has a width w , an outer diameter c , septa of thickness t and an inner diameter d . As a first approximation, we assume that the model geometry changes in a perfectly kinematically reversible, simple sinusoidal, manner. That is, all lengths change as $L(t) = \bar{L}R(t)$, where $R(t) = 1 + K \sin nt$, $K = (\varphi - 1)(\varphi + 1)$, $\varphi = (1 + C)^{1/3}$, $C = V_T/V_{FRC}$, $n = 2\pi/T$, V_T is the tidal volume, V_{FRC} is the lung volume at functional residual capacity, T is the

breathing period and the over bar signifies the mean value. For quiet breathing, $T = 4\text{s}$ and $C = 0.2$ (Weibel, page 284, [12]).

Flow and geometrical characteristics

The flow parameters we consider are the ratio of flow entering the alveolus to that passing by the alveolar opening in the duct, Q_A/Q_D (Fig. 3) and the Reynolds number of the flow in the duct, Re . The geometric parameters are the alveolar aspect ratio, $R_A = h/w$, where $h = (c - d)/2$; and the ratio of the depth to the inner duct diameters, $R_D = h/d$ (Fig. 3). We concentrate on the geometric configuration of $R_A = 1$ and $R_D = 0.5$. We also consider the effect of the alveolar shape by changing the outer alveolar surface from flat to peaked (Fig. 3b).

As we have assumed that the geometry remains similar at all times, Q_A/Q_D is simply a function of model geometry. Specifically, $Q_A/Q_D = V_A/V_D$, where V_A is the volume of the alveolus and V_D is the total acinar volume distal of the proximal septum of the alveolus of interest (Fig. 3). The value of V_D defines in which generation the alveolus of interest is located. We note that Re and Q_A/Q_D are linked through V_D . Specifically, we define $Re = U_{\max} \bar{d} / \nu$, where, $U_{\max}$ is the maximum bulk velocity, and hence, $Re = 6K\bar{V}_D / \nu T \bar{d}$. We see that the Reynolds number is a function of the tidal volume, V_T (through K), and the breathing frequency, $1/T$. Nonetheless, despite the fact that Re and Q_A/Q_D are both functions of V_D , Re has little affect on the flow in the alveolus. Conversely, the flow structure occurring in the alveolus is almost exclusively controlled by the value of Q_A/Q_D .

Governing equations

The Navier-Stokes equations, in cylindrical coordinates, were transformed into an equation for the transport of vorticity. An equation for the streamfunction was derived from the continuity equation. The vorticity and streamfunction equations were discretized on a moving mesh using the finite volume method. The resulting equations were solved on a multi-block grid using the line-by-line Gauss-Seidel method with implicit time marching. More details of the numerical methods employed can be found in the appendix.

Fluid particle tracking

Lagrangian fluid particle trajectories, $X(t)=(z,r)$, were computed in a stationary computational space from the resulting discrete (Eulerian) velocity field $u(x_i)=(u_z, u_r)$ by integrating numerically $dX=udt$, $X(t=0)=X_0$, where X_0 denotes an initial position. The fourth-order Runge-Kutta method was used to perform the integration. The local fluid particle velocity was estimated from the discrete velocity field using bilinear interpolation in space and cubic splines in time (Press, et al., [13]). The scheme is similar to the one used in Henry et al. [5] but here, because the grid was moving, it was more convenient to use the flow velocities (mapped onto the stationary computational space) in the Runge-Kutta scheme rather than the gradients of streamfunction. This, theoretically, introduces a small error to the resulting particle paths but we reduced the time-step until the tracks were essentially time-step independent.

Validation

There are no analytical solutions for flow in an expanding alveolated duct with which to test our predictions. Nonetheless, we ensured that our results were grid and time step independent. As the flow is quasi-steady for all physiological relevant breathing patterns, a relatively large time step ($T/48$) could be used without loss of accuracy.

We did test our numerical model against Uchida and Aoki's [14] exact similar solution for unsteady flow in a semi-infinite expanding tube. The appropriate Reynolds number, α , for

this flow is based on the wall velocity; i.e., $\alpha = a_0(da/dt)_0/\nu$, where, a is the tube radius and the subscript 0 defines the initial value. The wall Reynolds number for a typical acinar airway and quiet breathing is very small ($\sim 3 \times 10^{-5}$) and hence the expansion for low Reynolds number, given Uchida and Aoki [14], may be used. While the expansion in Uchida and Aoki's model is only in the radial direction, this solution is useful in testing various features of the program. The numerical model was applied to this flow using a two-block grid. Agreement between the prediction and analytical solution was excellent (Fig. 4).

RESULTS

We can view acinar flow as being composed of two distinct regions: (i) a central channel (i.e., the acinar duct) through which respiratory gases and particles are transported towards the terminal sacs and, (ii) numerous dead-ended side pockets (i.e., alveoli), surrounding the central channel, in which gas exchange takes place and the majority of deposition occurs. The focus of this study is the transport between these two regions. By the nature of the acinar airway geometry, this transport is largely in the radial (i.e., cross-stream) direction. In the following, we present results of computations in model alveoli, both rigid and expanding, that show how the rate of radial transport of momentum changes from the acinar entrance to the terminal ducts and how this affects the resulting acinar flow.

Following our approach in the Theoretical Considerations section, we considered the rate at which total momentum (per unit volume) is transported, by convection and diffusion, across the opening of the alveolus (shown as a broken line in the streamline maps of Fig. 5) over inspiration. As before, we divided the total momentum into axial, ρu_z and radial ρu_r components. Hence, the rates at which these components are transported in the radial direction convectively are $u_r(\rho u_z)$ and $u_r(\rho u_r)$, respectively, and diffusively are $-\nu(\rho u_z)/r$ and $-\nu(\rho u_r)/r$, respectively. Values of the velocity components and their radial gradients were computed by linear interpolation in the radial direction. In the expanding case, the line across the alveolar opening has a positive radial velocity. Hence, to correctly calculate the amount of flow crossing this line and entering the alveolus it was necessary to subtract the line's velocity from the predicted flow velocities (on a moving mesh, the predicted flow velocities include the mesh velocity). At each time step, the total of each component entering the alveolus was estimated by trapezoidal integration of the relevant terms along the line. The four components of radial transport of momentum (per unit density) across the opening of the alveolus were compared at each acinar generation at maximum inspirational flow rate; i.e., $t = T/4$ (Figs. 6 and 7).

First, it is evident that the rates of radial diffusional transport (Fig. 7) are in general much larger than the rates of radial convective transport throughout the acinar tree (Fig. 6). This is not a surprise since the Reynolds number of acinar flow is generally less than unity, which suggests that acinar flow is dominated by viscous forces. Furthermore, while the peak values of the diffusional transport rates between axial and radial momentums are comparable, their net values are fundamentally different. This is because while the rate of diffusional transport of axial momentum ($-\nu(\rho u_z)/r$) remains positive over the entire alveolar opening, the rate of diffusional transport of radial momentum ($-\nu(\rho u_r)/r$) varies from positive to negative across the opening of the alveolus (see below for further explanation).

At generation 15 (i.e., at the entrance of the acinus), the rate of diffusional transport of axial momentum ($-\nu(\rho u_z)/r$) was by far the largest component compared with other components (Fig. 7). Because the sign of the radial velocity changes (from positive to negative) along the alveolar opening, the net transport of axial momentum by convection was essentially zero. For similar reasons, the net diffusional transport of radial momentum was also close to zero. There was, however, a net inflow of radial momentum but the rate of

this was extremely small compared to the rate of diffusional transport of axial momentum. As expected, from the similarity in streamline patterns (Fig. 5), the curves of transport for the expanding and rigid models of generation 15 were predicted to be identical.

The variation across the alveolar opening of the rates of radial transport for generations 17 (not shown) and 19 were found to be similar to those for generation 15 but the magnitudes of each curve reduced with generation number. At generation 21, the reduction in axial momentum in the duct was such that the rotation in the alveolus was confined to the proximal half of the alveolus (Fig. 5). The curves of convective transport across the opening (Fig. 6) show the effect of this reduction in alveolar rotation in that more momentum, both radial and axial, is drawn into the proximal half of the alveolus compared to the distal half. However, convective transport is still negligible compared to the diffusive transport of axial momentum. At generation 23, the variation of convective transport predicted by the rigid model is noticeably different from that predicted by the expanding model.

At generation 23, convective transport is positive across the entire alveolar opening for both axial and radial momentum (Fig. 6). Again, however, the rate of convective transport is negligible compared to diffusional transport. It is noted that diffusional transport is still predicted to be negative over about a third of the alveolar opening (Fig. 7). In addition, while the variation of diffusional transport is somewhat similar, the variation of convective transport predicted by the rigid model is obviously different to that predicted by the expanding model. Hence, while the dominating transport mechanism for momentum; i.e., diffusional transport, is predicted to be similar in both rigid and expanding models, the streamline patterns produced by these models are completely different. This has important implications for the transport of particles with little intrinsic motion (i.e., low diffusivities) in the lung periphery. Specifically, it can be inferred from the right-most panels of Fig. 5, that the rigid model would predict that the particle travels along a counter-clockwise rotating path and the expanding model would predict that the particle travels in a radial direction.

To compare our predictions with the order-of-magnitude estimates (Fig. 2), we computed the rate at which axial and radial momentum were transported, by convection and diffusion, across the alveolar opening at each time step over inspiration. That is, at each time step, we approximated numerically the four integrations given by equations 1–4. We then computed the time average of each of the four components of momentum transfer entering the expanding alveolus over inspiration, using trapezoidal integration in time, for each generation (Fig. 8). Again, to aid in the comparison to the curves in as in Fig. 2, we present the results in terms of the ratios R_1 , R_2 and R_3 . That is, we divided the convection and diffusion of radial momentum and the convection of axial momentum by the diffusion of axial momentum. We found that, i) diffusion of radial momentum (Fig. 8) increases more than 2 orders of magnitude along the acinar tree and becomes comparable to diffusion of axial momentum at the terminal alveolar sacs (generation 23). This is as expected as the flow Reynolds number is approaching zero in this region and hence Stokes' flow prevails. ii) convection of radial momentum (Fig. 8), while small even at generation 15 compared to diffusion of axial momentum, decreases by 100 folds from generation 15 to generation 21 and remains low in the remaining generations. Inspection of the curves for radial convection of radial momentum at generation 15 and generation 23 (Fig. 6) reveals that while the transport is always positive it reduces in magnitude relative to diffusional transport and this trend is seen in the curve of total transport (Fig. 8). We note that, in general, the trends predicted here agree with those estimated using the order-of-magnitude arguments (Fig. 2). However, the magnitude of the radial convection of axial momentum is predicted to be considerably lower than that given by the order-of-magnitude estimate. The most plausible explanation for this difference is that the actual mean value of axial velocity along the alveolar opening is much smaller than the mean velocity in the duct.

The results presented above show that the magnitude of the axial momentum in the duct is the critical factor in determining the nature of the flow in the surrounding alveoli. In the above analysis, we have used the Eulerian approach. Another way to assess the flow in the alveolus is to use the Lagrangian approach; i.e., to follow typical fluid elements within the alveolar flow. To this end, we computed the paths of fluid elements over inspiration starting from the same initial position (midway along the alveolar opening) in each alveolus (Fig. 9). We found that, over inspiration, the fluid element in generation 15 made approximately eight revolutions of the alveolus and that the number of revolutions roughly halved for each subsequent generation so that the fluid element in generation 18 made approximately 1–1/4 revolutions. From generation 19 on, the fluid element only travels a fraction of a revolution and the direction of the pathline becomes increasingly more radial. At generation 23 there is no indication of rotational flow; i.e., the pathline is essentially radial.

In order to quantify the strength, or intensity, of the alveolar flow, we computed the total length of the path taken by a fluid element over inspiration, I , with generation number, n (Fig. 10). That is, we assume that this length is proportional to the average intensity of the alveolar flow over inspiration; i.e., we assume that $I = u_A \times T/2$, where u_A is proportional to the average, over inspiration, of the square root of the kinetic energy of the alveolar flow. We see that, in general, the path length decreases with increasing generation number. While at first glance, the curve of I versus n appears to follow a simple exponential decay, on closer inspection the curve is seen to have two distinct regions. Specifically, over generations 15 through 19, the time constant of decay is predicted to be 1.454, while over generations 20 through 23 it is predicted to be 3.173 (Fig. 10). In addition, we see that I/w is roughly an order of magnitude larger in the entrance region of the acinus than in the periphery.

The results of the above momentum transfer analysis and the predicted paths of fluid elements show how particles might behave once they have entered the alveolus. However, such analysis cannot explain the manner in which particles with little intrinsic motion enter the alveolus. Nonetheless, as the alveoli are expanding over inspiration, we know that particle-laden air must enter the alveolus over inspiration. That is, an application of the principle of the conservation of mass shows that air, being incompressible, must always completely fill the alveolar volume and as the volume is increasing; air from the duct must enter the alveolus over inspiration.

To see where, over the alveolar opening, the air enters the alveolus we compared the convective flow paths in a region of the alveolar opening near the distal septa wall predicted by the expanding model to those predicted by the rigid model (Fig. 11). The pathlines started at the same initial position but diverged near the distal septal wall. The pathlines in the rigid-wall model (broken lines in Fig. 11) travel toward the distal generations without being able to enter the alveolus; whereas, the pathlines in the expanding-wall model (solid lines in Fig. 11) enter the alveolus, being exposed to the rotating flow structure existing inside the alveolus. These computations suggest that, due to the counter-clockwise rotational motion of the alveolar flow over inspiration, the particle-laden air is forced to enter the alveolus through a small portion of the alveolar opening near the distal septum.

We also used the Lagrangian approach to investigate the dispersion of particles once they enter the alveolus. Specifically, we followed two fluid elements over ten breathing cycles (Fig. 12, upper panels). At the beginning of the first breath, the particles were placed midway along the alveolar opening. The particle pairs were initially separated by a distance equal to 0.01% of the septa width. It was found that the distance separating the two particles changed appreciably over each breathing cycle and that the pattern of this change was not constant from cycle to cycle (Fig. 12, lower panels).

DISCUSSION and CONCLUSION

Flow momentum

The strength of alveolar rotational flow has been shown to be intimately linked to the magnitude of the axial momentum of the central channel flow. Specifically, we have shown that the principal way in which the axial momentum affects the alveolar flow is by radial viscous diffusion. That is, as the kinematic viscosity of a fluid, ν , can also be thought of as a diffusivity for momentum, the transfer of momentum from the central duct flow to the alveolar flow is by diffusion down the gradient of axial momentum ($\rho u_z / r$). We note that as the flow in the alveoli is rotating slowly relative to the flow in the channel then $\rho u_z / r$ will always be negative across the alveolar opening and hence the direction of axial momentum transfer will always be from the duct to the alveolar flow. Our curves of the variation of u_z / r over the alveolar opening (Fig. 7) confirm this conclusion.

When the flow in the alveolus rotates, its momentum changes from being mostly axial, as it travels past the alveolar opening and on its return over the septal surface opposite the opening, to being generally radial, as it travels up and down the distal and proximal septa. Thus there is created a gradient of radial momentum ($\rho u_r / r$) and hence the possibility of diffusion of radial momentum in the radial direction. Our results (Fig. 7) indicate that such diffusional transport occurs and that the absolute magnitude of the diffusion of radial momentum is comparable to that for the diffusion of axial momentum. However, due to the change in sign of the gradient of radial momentum over the alveolar opening, the net transport into the alveolus of radial momentum is close to zero. Somewhat surprisingly, even when there is not recirculating flow (i.e., in generation 23) there is still a sizable portion of the alveolar opening for which the direction of diffusional transport of radial momentum is from the alveolus to the duct (Fig 7).

In the expanding model, there is a positive radial flow into the alveolus over inspiration. Thus, this radial flow will carry (convect) momentum from the duct flow into the alveolus. When the flow rotates, the flow entering from the duct is forced to do so over a small portion of the alveolar opening located near the distal septum (Fig. 11). Thus while the volume flow into the alveolus, Q_A , is small relative to that passing by the opening in the duct, Q_D (i.e., Q_A/Q_D is small for but the terminal ducts) the velocity of the flow entering the alveolus, over a small part of the opening, will be higher than would be the case if the volume flow entered evenly over all the alveolar opening. Evidence of this positive radial transport can be seen in the curves of convection of axial and radial momentum for generations 19 and 21 (Fig. 6). Specifically, the distal parts of these curves for the expanding models have smaller (negative) maximums than the comparable curves for the rigid models. That is, the radial velocity along the line on which the momentum transport is computed (the broken line in Fig. 5) is less negative near the distal septum in the expanding model than in the rigid case because of the positive radial velocity in that area caused by the expanding alveolus. At generation 23, which has no rotation, the direction of radial convection of both axial and radial momentum is into the alveolus over all of the alveolar opening.

While the expansion of the alveolus does cause convective transport of momentum, from the duct flow into the alveolar flow, our results show that its contribution is negligible relative to that of diffusional transport. At the entrance to the alveolus (generation 15), convection of radial momentum is highest but even then is only 1000th of that due to diffusional transport (Figs. 6 and 7). The rate of radial convection of axial momentum is lower still. As the flow travels towards the terminal ducts, the effect of convective transport drops further. This last result is in keeping with the fact that Re in the terminal duct is close to zero and hence diffusional transport dominates.

We note that the strength of the recirculation in the alveolar flow is directly related to the strength of the axial momentum in the duct. That is, the rate of viscous diffusion, which is proportional to the kinematic viscosity, ν , is relatively constant throughout the acinus but the strength of the quantity being diffused; i.e., the axial momentum, reduces by half for each generation and at the terminal duct has reduced to the point where rotation in the alveolus can no longer be maintained.

Acinar flow

Our results show that some degree of recirculation occurs in all but the terminal generations. Thus, we can divide the acinus into two regions; i.e., the proximal region, in which the alveoli have some level of recirculating flow, and the distal region, in which there is no recirculation and the flow is largely radial in direction. Our group has previously found similar results for more fully 3D models of alveoli (Haber et al., [6]). In addition, more recently, others have presented comparable findings (Snitzman et al., [8], Kumar et al., [9] and by Darquenne et al., [9]). We note that the streamline patterns predicted by our axisymmetric model are similar to those in the symmetry planes of the 3D models. In addition, the main characteristic of alveolar flow in the entrance region of the acinus is that of rotation about an axis at 90° to the main duct flow and the main feature of the flow in the peripheral alveoli is that the flow is mainly radial. Both characteristics are predicted by our model. Thus while our model does not predict the secondary, cross stream (circumferential), features of alveolar flow it does capture the fundamental characteristics of these flows.

We have shown that the strength of recirculation increases exponentially with decreasing generation number (Figs. 9 and 10). In addition, Q_A/Q_D decreases exponentially with decreasing alveolar generation number (Fig. 2). Recently, Henry et al., [5] showed that increasing the duct Re in a rigid model, which is equivalent to decreasing Q_A/Q_D in an expanding model, appears to increase the area of chaos in the alveolus. Hence, we can expect that the amount of chaotic mixing increase as the acinar entrance is approached. An indication of the mixing characteristics of alveolar rotating flow has been given by the plot of the time evolution of the distance between two particles as they travel around the alveolus (Fig. 12). This plot shows how the distance between two fluid elements can change substantially over an individual breathing cycle and from one cycle to another.

These results together with the analysis of Henry et al., [5] leads us to the conclusion that the acinus can be considered as containing millions of tiny mixing units with a range of mixing strengths.

Physiological implications

It has been repeatedly demonstrated that the proximal region of the acinus is the primary site of particle deposition and lung injury after exposure to airborne pollutants (Pinkerton et al., [15]; Saldiva et al., [16]). For instance, Churg and Brauer [17] reported that submicron size particles were found at the entrance of the acinus at typically 25–100 times higher concentration than in the main stem bronchi. Our results indicate that alveolar flow rotation, and by implication chaotic mixing, are strongest in the entrance generations. Our results also show that the expanding alveolus provides a pathway by which particles with little intrinsic motion can enter the alveoli. We note that particles in the range of 0.1 to $1.0 \mu\text{m}$ are little affected by gravity (gravity numbers, $H_g = 4 \times 10^{-3}$ to 2×10^{-1}), inertia (Stokes numbers, $Stk = 10^{-7}$ to 10^{-6}), or Brownian motion (diffusivities of particles in this range are 10^{-5} to 10^{-6} times smaller than the diffusivity of oxygen molecules in air). Thus, our results offer a possible explanation for why submicron particles deposit preferentially in the acinar entrance region. Specifically, such particles are drawn into the alveolus by the expanding alveolar geometry where they enter the rotational flow and are mixed and eventually

deposited by chaotic convection. Finally, we note that there is a view (see for instance Kitaoka et al. [18]) that in a normal healthy lung, the size of the alveoli do not change significantly during inspiration and expiration, and that the expansion of the ducts essentially accounts for the tidal volume. However, as far as we know, a consensus on this point has not been reached.

Acknowledgments

This study was supported by NIH Grants HL054885, HL070542 and HL074022.

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APPENDIX

Governing equations

The equation for the transport of vorticity in cylindrical polar coordinates can be written as

$$\frac{\partial \zeta}{\partial t} + \frac{\partial}{\partial z}(u_z \zeta) + \frac{\partial}{\partial r}(u_r \zeta) = \nu \nabla^2 \zeta - \nu \frac{\zeta}{r^2} \quad (\text{A1})$$

where $\zeta = u_r / z - u_z / r$ and $\nabla^2 \varphi = \frac{\partial^2 \varphi}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \varphi}{\partial r} \right)$

The Stokes streamfunction, ψ , is defined as (Batchelor, page 78, [19])

$$u_z = \frac{1}{r} \frac{\partial \psi}{\partial r}, \quad u_r = -\frac{1}{r} \frac{\partial \psi}{\partial z} \quad (\text{A2})$$

An equation relating the Stokes streamfunction to the vorticity is derived by substituting equations A2 into the continuity equation and rearranging to give

$$\nabla^2 \psi = 2u_z - r\zeta \quad (\text{A3})$$

Numerical discretization on a moving grid

Each term in equations A1 and A3 was integrated over a typical grid cell of volume V_P (Fig. A1). Gauss' theorem and the mid point rule were invoked in the integration of the derivative terms (Ferziger and PeriS, [20]).

In the case of a grid that moves and expands in time, the time term in the transport equation has to be integrated with the aid of Leibniz rule; i.e.,

$$\iiint_{\Delta V} \frac{d\varphi}{dt} dV = \frac{d}{dt} \iiint_{\Delta V} \varphi dV - \iint_S \varphi \frac{d\mathbf{r}}{dt} \cdot \mathbf{n} dS$$

For an expanding axisymmetric polar grid, $\theta = \theta(t)$ and hence we can write

$$\frac{d\mathbf{r}}{dt} = \frac{dr}{dt}\mathbf{i}_r + \frac{dz}{dt}\mathbf{i}_z = \mathbf{v} = v_r\mathbf{i}_r + v_z\mathbf{i}_z$$

Hence, assuming that the cell is one radian thick in the circumferential direction, the time term on a moving grid approximates to

$$\begin{aligned} \frac{\partial}{\partial t} \iiint_{\Delta V} \zeta dV - \iint_S \zeta \mathbf{v} \cdot \mathbf{n} dS \approx & V_p \frac{\partial}{\partial t} \zeta_p + \zeta_p \frac{\partial}{\partial t} V_p - [(v_z)_e S_e^z + (v_r)_e S_e^r] \zeta_e - [(v_z)_n S_n^z + (v_r)_n S_n^r] \zeta_n \\ & - [(v_z)_w S_w^z + (v_r)_w S_w^r] \zeta_w - [(v_z)_s S_s^z + (v_r)_s S_s^r] \zeta_s \end{aligned}$$

$$\begin{aligned} S_e^z &= r_e (r_{ne} - r_{se}), S_n^z \\ &= r_n (r_{nw} - r_{ne}), S_w^z \\ &= r_w (r_{sw} - r_{nw}), S_s^z \\ &= r_s (r_{se} - r_{sw}), S_e^r \\ &= r_e (z_{se} - z_{ne}), S_n^r \\ &= r_n (z_{ne} - z_{nw}), S_w^r \\ &= r_w (z_{nw} - z_{sw}), S_s^r \end{aligned}$$

where $= r_s (z_{sw} - z_{se})$ (see Fig. A1).

Hence, the integration of the left-hand side of the transport equation (eqn. A1) over a typical moving and expanding cell is approximated as

$$\begin{aligned} \iiint_V \frac{\partial \zeta}{\partial t} dV + \iiint_V \frac{\partial}{\partial z} (u_z \zeta) dV + \iiint_V \frac{\partial}{\partial r} (u_r \zeta) dV \approx & V_p \frac{\partial}{\partial t} \zeta_p + \zeta_p \frac{\partial}{\partial t} V_p \\ & + [(u_z - v_z)_e S_e^z + (u_r - v_r)_e S_e^r] \zeta_e + [(u_z - v_z)_n S_n^z + (u_r - v_r)_n S_n^r] \zeta_n \\ & + [(u_z - v_z)_w S_w^z + (u_r - v_r)_w S_w^r] \zeta_w + [(u_z - v_z)_s S_s^z + (u_r - v_r)_s S_s^r] \zeta_s - (\mu_r \zeta)_p \Delta A_p \end{aligned}$$

where, ΔA_p is the cross-sectional area of cell P (Fig. A1).

The diffusion terms in eqns. A1 and A3 are integrated over the typical cell to give

$$\iiint_V \nu \left[\frac{\partial^2 \varphi}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \varphi}{\partial r} \right) \right] dV \approx \nu \left(\frac{\partial \varphi}{\partial n} \right)_e S_e + \nu \left(\frac{\partial \varphi}{\partial n} \right)_n S_n + \nu \left(\frac{\partial \varphi}{\partial n} \right)_w S_w + \nu \left(\frac{\partial \varphi}{\partial n} \right)_s S_s$$

The velocities at the center of the cell, are assumed to represent the cell-averaged values; i.e.,

$$(u_z)_p = \bar{u}_z = \frac{1}{\Delta V} \iiint_V \frac{1}{r} \frac{\partial \psi}{\partial r} dV \approx \frac{1}{V_p} \left(\psi_e \frac{S_e^r}{r_e} + \psi_n \frac{S_n^r}{r_n} + \psi_w \frac{S_w^r}{r_w} + \psi_s \frac{S_s^r}{r_s} \right)$$

and

$$(u_r)_p - \overline{u_r} = -\frac{1}{\Delta V} \iiint_V \frac{1}{r} \frac{\partial \psi}{\partial z} dV \approx -\frac{1}{V_p} \left(\psi_e \frac{S_e^z}{r_e} + \psi_n \frac{S_n^z}{r_n} + \psi_w \frac{S_w^z}{r_w} + \psi_s \frac{S_s^z}{r_s} \right)$$

The remaining terms in eqns. A1 and A3 were integrated as follows-

$$\iiint_V v \frac{\zeta}{r^2} dV \approx v \frac{\zeta_p}{r} A_p, \quad \iiint_V 2u_z dV \approx 2(u_z)_p V_p \quad \text{and} \quad \iiint_V r \zeta dV \approx r_p \zeta_p V_p$$

The time derivative is approximated using two-point backward Euler differencing. Cell face values of vorticity were approximated using deferred-correction central differences (Ferziger and PeriS, [20]). The gradients of vorticity and streamfunction at the cell faces were approximated using central differences with a deferred correction scheme suggested by Muzaferija [21] to avoid oscillations that occur in the solution due to the use of central differences on a collocated grid.

The above approximations require that the value of a variable and its gradient are known at the mid point of a cell face but in the finite volume method, values are only known at the center of each cell. In an orthogonal grid, the value of a variable at the mid point of a cell face is taken to be the weighted average of the values of the variable at the center of the two cells either side of the cell face. Similarly, the gradient of the variable at the cell face is approximated using the same two cell-center values. In the case of an irregular and non-orthogonal grid, the mid point of a cell face does not lie, in general, on the line between cell centers. A scheme suggested by Ferziger and PeriS, (page 225, [20]) was used to estimate the cell face values and gradients using additional cell values. Terms containing the additional cell values were added to the source term so that the usual five-point solution module was maintained. The resulting implicit discrete equations were solved on a multi-block grid (Fig. A2) using the line-by-line Gauss-Seidel method and the tri-diagonal matrix algorithm with under-relaxation.

Grid motion

The equation of space conservation can be given as

$$\frac{\partial}{\partial t} \iiint_{\Delta V} dV - \iint_S \mathbf{v} \cdot \mathbf{n} dS = 0 \quad (\text{A4})$$

Using the Gauss' theorem and the mid point rule, the discrete version of eqn. A4, can be written as

$$\frac{d}{dt} (\Delta V_p) = (v_z)_e S_e^z + (v_r)_e S_e^r + (v_z)_n S_n^z + (v_r)_n S_n^r + (v_z)_w S_w^z + (v_r)_w S_w^r + (v_z)_s S_s^z + (v_r)_s S_s^r$$

The above equation must be satisfied exactly if artificial mass sources are to be avoided. The difference scheme used to model the face velocities is critical in this regard. For instance, Demirdži and Peri [22] demonstrated that the two-point explicit formula for grid velocity;

i.e., $(v_z)_e = (z_e^{t+\Delta t} - z_e^t) / \Delta t$, does not, in general, ensure space conservation. Fortunately, in the present case, we do not have to use finite differences to estimate the cell face velocities because we define the grid position analytically ($z(t) = \bar{z}F(t)$ and $r(t) = \bar{r}F(t)$) and hence can also define analytical expressions for the face velocities ($v_z(t) = \bar{z}dF/dt$ and $v_r(t) = \bar{r}dF/dt$) and cell volumes ($\Delta V = 3\bar{\Delta}\bar{V}F dF/dt$). Using consistent analytical expressions ensures that the discrete space conservation equation is satisfied exactly.

Boundary conditions

Inlet and outlet

We define quasi-periodic axial boundary conditions on the streamfunction and vorticity. Essentially, we assume that the added volume flow rate between model inlet and outlet, due to the expanding geometry, results in an additive velocity at the inlet that is parabolic with the radial direction. Specifically,

$$\psi_{inlet,j} = \psi_{outlet,j} + \left[\frac{24\bar{V}}{\bar{d}^2} \bar{r}_j^2 \left(1 - \frac{\bar{r}_j^2}{\bar{d}^2} \right) - (\bar{z}_2 - \bar{z}_1) \frac{\bar{r}_j^2}{2} \right] F^2 \frac{dF}{dt}$$

and

$$\zeta_{inlet,j} = \zeta_{outlet,j} + \frac{384\bar{V}}{\bar{d}^4} \frac{1}{F} \frac{dF}{dF} \bar{r}_j$$

where the overbar defines average values. We define the streamfunction at the intersection of the outlet plane and the duct wall as $\psi_{outlet,j_{max}} = \psi_{outlet,wall} = 3 V_{distal} \bar{r}^2 dF/dt$, where V_{distal} is acinar volume distal of the model. Values of V_{distal} were chosen to produce flow conditions in the middle alveolus that are typical of alveoli in specific areas of the acinus.

Values of the velocity components, u_z and u_r along the inlet and outlet plane were estimated by extrapolation from the interior solution.

The above scheme is mass conservative but may introduce a small inaccuracy in the inlet and outlet velocity profiles. Nonetheless, we have taken steps to reduce the influence of any such inaccuracy by computing the flow in three alveoli in series and concentrating our analysis on the middle alveolus. As the Reynolds number is low (i.e., viscous diffusion of momentum is rapid), the velocities can be expected to adjust to the correct profiles over a distance of one alveolar width.

Walls

Unlike the rigid case, the streamfunction along a moving wall is not constant. Nonetheless, as we have analytical expressions for the change of geometry with time it is possible to define the streamfunction along any solid surface of the model. That is, between any two points along a solid surface

$$\psi_2 - \psi_1 = \int_1^2 r u_z dr - \int_1^2 r u_r dz = F^2 \frac{dF}{dt} \left(\int_1^2 \bar{r} \bar{z} d\bar{r} - \int_1^2 \bar{r}^2 d\bar{z} \right)$$

Before each time step the above integration is performed over each grid cell coincident with the solid surface starting at the outlet, where $\psi_1 = 3 V_{distal} F^2 dF/dt$.

The vorticity at the wall has to be found iteratively. The formula used to update the vorticity before each iteration is derived from the definition of vorticity; i.e., $\zeta = u_r/z - u_z/r$. This equation is first transformed by chain differentiation into one in which the derivatives are with respect to local coordinates parallel, s , and normal, n , to the surface (Fig. A3); i.e.,

$$\zeta = \left(\frac{\partial u_r}{\partial s} - \frac{\partial u_z}{\partial n} \right) \cos \sigma - \left(\frac{\partial u_r}{\partial n} + \frac{\partial u_z}{\partial s} \right) \sin \sigma$$

Where σ is the angle made by the wall surface (positive s -direction) and the positive z -axis (Fig. A3). Equations A2 are then used together with more chain differentiation to transform the above equation into an equation relating vorticity to gradients of streamfunction in the s and n directions. As the streamfunction and velocities are known analytically along the wall (s -direction) all terms in the resulting equation are known except $(\partial^2 \psi / \partial n^2)_w$, which is approximated using a truncated Taylor series. The resulting equation for the wall vorticity can be written as,

$$\zeta_w = -2 \frac{\psi_1 - \psi_w}{\bar{r}^2 (\Delta \bar{n})^2 F^3} + \frac{1}{r} \left[(2\bar{z} - \bar{r}) \cos \sigma \sin \sigma + \bar{z} \cos^2 \sigma + \frac{2\bar{r}}{\Delta \bar{n}} (\bar{r} \sin \sigma + \bar{z} \cos \sigma) \right] \frac{1}{F} \frac{dF}{dt}$$

Where, ψ_1 is the value of the streamfunction at the center of the cell coincident with the wall, ψ_w is the value of the streamfunction at the mid point of the cell face on the wall surface, and Δn is the distance between cell center and cell face midpoint (Fig. A3). Before each iteration of the vorticity equation, ψ_1 is updated using the current streamfunction solution. We note that in the rigid case the above formula reduces to that recommended by Roache (page 151, [23]).

Centerline

The streamfunction is constant along the centerline and can be set to zero without any loss of generality. The vorticity and radial velocity are identically zero along the centerline. The axial velocity along the centerline is unknown and is found iteratively by extrapolation and assuming a parabolic distribution of velocity in the vicinity of the centerline.

Implementation of boundary conditions

A halo of dummy cells was created around each grid block to facilitate in the application of boundary conditions. In the case of inter-clock boundaries, the value of a variable in a dummy cell was given by the corresponding cell in the neighboring grid block. In the case of actual boundary conditions, the dummy cell value was determined by extrapolation using the appropriate boundary condition on the solution boundary surface and the value of the variable in the interior cell coincident with the surface and adjacent to the dummy cell.

Figure A1.
Typical non-orthogonal grid cell

Figure A2.
5-block grid. Broken lines indicates block boundaries

Figure A3.
Wall boundary cell.

(a) Scanning electron micrograph of an alveolar duct surrounded by alveoli (From Gehr et al. [24], by permission). (b) Schematic of dichotomously bifurcating acinar airways.

Figure 2.
Estimated variation of convective and diffusive radial transport of radial and axial momentum, over inspiration, normalized by diffusive radial transport of axial momentum. Included are the variations of Re at maximum inspirational flow rate and QA/QD.

Figure 3.

(a) Three-alveoli solution domain: Q_A is the volume flow into the alveoli and Q_D is the volume flow in the duct. (b) 3D cross-sectional view of solution domain (with peaked top surface).

Figure 4. Prediction and analytical solution (Uchida and Aoki, [14]) of flow in an expanding tube.

Figure 5.

Predicted streamlines for expanding (upper) and rigid (lower) model alveoli for generations 15, 19, 21 and 23. The broken line shown in the lower left panel indicates the line along which transport into all alveoli is calculated.

Figure 6.

Rate of radial convective transport of axial momentum, per unit density, ($u_r u_z$) and rate of radial convective transport of radial momentum, per unit density, ($u_r u_r$) along the alveolar opening (i.e., along the broken line in the lower left panel of Fig. 5) at maximum inspirational flow rate; i.e., $t = T/4$, for expanding (upper) and rigid (lower) model alveoli for generations 15, 19, 21 and 23.

Figure 7.

Rate of radial diffusive transport of axial momentum, per unit density, $(-\nu u_z / r)$ and rate of radial diffusive transport of radial momentum, per unit density, $(-\nu u_r / r)$ along the alveolar opening (i.e., along the broken line in the lower left panel of Fig. 5) at maximum inspirational flow rate; i.e., $t = T/4$, for expanding (upper) and rigid (lower) model alveoli for generations 15, 19, 21 and 23.

Figure 8.
Predicted total radial transport over inspiration normalized by total radial diffusion of axial momentum over inspiration.

Figure 9.

Typical paths taken by fluid elements over inspiration in model alveoli in each alveolar generation. Starting position denoted by the symbol $\odot$.

Figure 10.

Normalized distance traveled over inspiration by fluid elements in model alveoli in each generation. Distance (l) normalized by the alveolus width (w). Starting position of fluid elements in each alveolus as shown in Figure 9.

Figure 11.

Area near the proximal alveolar septum (shaded) over which flow enters the expanding model alveolus. The lower (broken) line is the path taken by a fluid element in the rigid model. The upper (solid) line is the path taken by the same fluid element in the expanding model.

Figure 12.

Path lines of a pair of fluid elements over ten breathing cycles (upper panels) and time history of the distance between the fluid elements, s , normalized by the alveolar width, w (lower panels). Initial position of fluid elements shown by the symbol $\odot$. Initial value of normalized separation, $s/w = 0.0001$.